Chemkin workshop panel questions / answers

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Experience in teaching

- **University of Maryland**
  - Undergraduate: Dynamics, Environmental Honors
  - Graduate: Combustion (twice)
- **University of California, San Diego (current)**
  - Undergraduate: Intro. to Mech. Eng., Non-Nuclear Energy Technologies, Experimental Techniques
  - Graduate: Fluid Mechanics I, Combustion
- **I have used Chemkin in a limited manner while teaching Combustion at University of Maryland for one problem set (out of 6) in the semester**

Combustion class syllabus (Fall 2002, UMCP)

Lecture	Topic	Reading (Glassman unless otherwise noted)	Assignment	
1	Introduction			
2	Combustion Thermodynamics	Chapter 1		
3	Transport properties, Basic Kinetic Theory + Arrhenius	Chapter 2 A, B		
4	Types of fundamental reaction, Hydrogen / Oxygen system, 1st, 2nd explosion limits	Ch 2 C-G, Ch 3 A-C		
5	CO / Methane combustion	Ch 3 D-H	**PS #1**	thermo and kinetics
6	Combustion models and their implemetation (PFR, PSR), examples	Appendix H, Chemkin documentation		
7	Modeling of higher hydrocarbons, model reduction, sensitivity analysis	Chemkin documentation, papers		
8	Conservation equations, conserved scalar analysis	notes, Turns		
9	Premixed Flames - Laminar	Ch 4 A-C		
10	Premixed Flames - Laminar	Ch 4 D		
11	Introduction to Turbulence	Ch 4 E, F		
12	Ignition and Extinction	Chapter 7	**PS #2**	chemkin
13	Ignition and Extinction			
14	Detonations - theory	Ch 5 A-C	**PS #3**	premixed flames
15	Detonation models	Ch 5 D-G		
16	Reaction modes, scaling, review		**PS #4**	ignition and extinction
17	Midterm - through lecture 13			
18	Nonpremixed flames - laminar	Ch 6 A, B		
19	Turbulent Nonpremixed Flames			
20	Burke-Schumann analysis	Handout		
21	Droplet Burning	Ch 6 C-E	**PS #5**	nonpremixed flames
22	Solid fuel combustion	Ch 9 A, C-F		
23	Solid fuel combustion	Ch 9 B		
24	Combustion Emissions - criteria pollutants, particulates and HAPS	Ch 8 A-E		
25	Combustion Emissions - reduction methods			
26	Combustion Diagnostics - basic	handouts		
27	Combustion Diagnostics - laser-based		**Project due**	
28	Review			
29	FINAL EXAM			

My approach to teaching Combustion

- In the past I've taught one-semester courses where this is typically the student's first (and only) exposure to combustion
- Stress the fundamentals
- Cover all of the basic problems
- Use basic tools where possible

➔ End goal: students should have the vocabulary of combustion, understand the breadth of problems and the standard approaches to these problems, have insight into the literature that would enable further study and/or research

➔ Final exam: ORAL

Integration of *CHEMKIN*

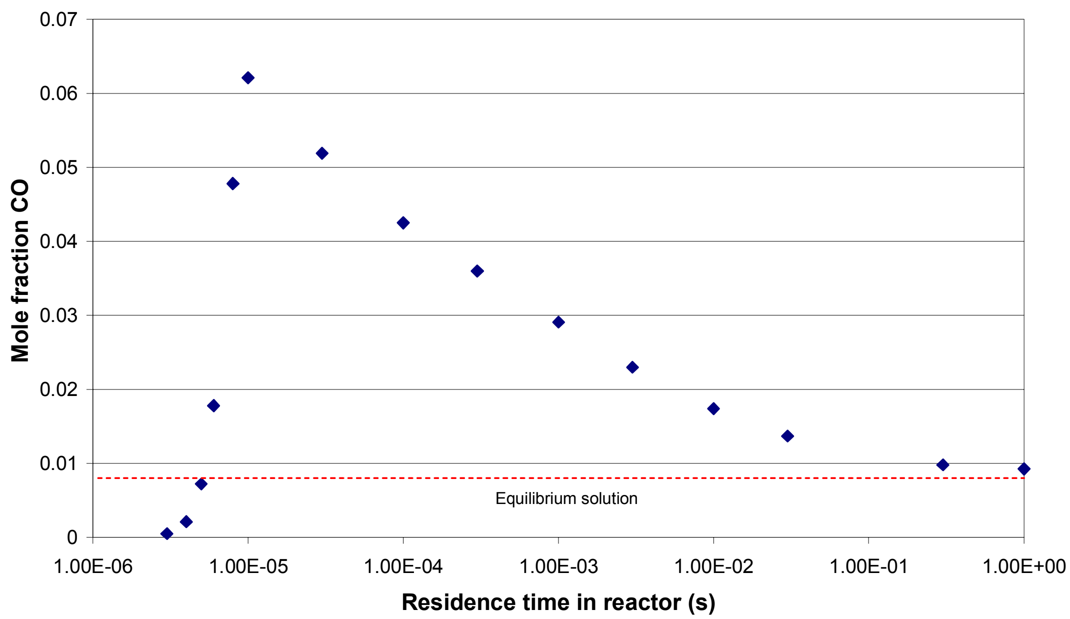
- **Typically confined to basic problems**
- **Investigation of kinetics**
  - Key reactions
  - Effect of temperature and pressure
- **Analogy of PSR / PFR combinations to progress of fluid parcels through a flame**
- **Using example problem, the effect of diluents on flame structure**

- **In the past I've introduced Chemkin early in the class and after this we have not used it, except as a component of one of two potential projects**

Example problem

Describe the problem that Aurora solves. Using Aurora, investigate the effect of residence time on CO emitted from a premixture corresponding to stoichiometric CH_4 / air. Set the reactor temperature equal to the adiabatic flame temperature, as calculated for your mixture from EQUIL. What might be some of the implications of your findings concerning the residence time / CO relationship for high-speed (high Re) flames? Look up "flame stretch" in your textbook for more information.

Aurora perfectly stirred reactor:
CO as a function of residence time, problem 3



- Well stirred reactor
- Often used to describe high-intensity combustion
- Flames have a distribution of residence times (RT)
- RT effects the completeness of combustion

Example project

- **Students had the choice of a “consultant-type” question or a theoretical question related to droplet burning**

➔ **“Chemical kinetic modeling is very important for the design of industrial burners, stationary gas turbines, and aircraft gas turbines, (maybe even H2/O2 rockets) both to predict performance and to predict emissions.**

  – Pick an actual system from the above list for which you can find or reasonably estimate some data (mass flow rates, pressures, degree of premixing, etc.)
  – Describe how you would construct a baseline model for this system using the (combination of) tools available in Chemkin. Your model will likely use more than one driver. Has this model been used before?
  – Exercise the model to predict performance (e.g. heat rate, power, thrust, whatever the important parameters are).
  – Compare your data with available performance data. How did you do?
  – Implement NOX control strategies – pick one – reburning, staged combustion, or ammonia injection. Describe both the method (background) and your results.
  – In reality, all real world systems have some degree of unsteadiness to them. Describe the effect of the unsteadiness on the system of your choice. Use PASR, if possible, to capture / estimate some of the effect of the unsteadiness.”

Primary benefits of Chemkin

- **Illumination of basic phenomena**
- **Clear illustration of kinetic limitations, equilibrium vs. kinetics, and effect of various kinetic mechanisms**
- **Variation of parameters over a wide range**

Biggest difficulties with using Chemkin

- Getting it up and running (this is no different from other software
- Massaging output into tractable forms for presentation

Source code issue

- **I don't have time to teach the numerical methods / programming aspect, and have not needed the source code.**
- **I've never used the API in the context of my class**
- **This is an active research issue, RD should address this**
  - May ultimately redound to the benefit of all (RD and users) to open the code